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CHEMICAL PROCESS OPTIMIZATION FOR DUMMIES

By Troy Mannino

A thesis submitted to the faculty of the University of Mississippi in partial fulfillment of the requirements of the Sally McDonnell Barksdale Honors College.

Oxford

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Abstract

Chemical process optimization is a daunting task. The purpose of this work is to summarize and organize successful approaches which may be employed by the chemical process engineer when confronted with optimization problems. In general, optimization is making any process better; common goals are to increase the efficiency or maximize the economic potential of a process. The improvements made to a process during optimization are generally measured in terms of an objective function. Since the purpose of any industrial chemical process is to be profitable, objective functions most often have units of dollars. The objective function is dependent upon changes in decision variables, those variables over which the engineer has control. The two most common approaches to optimization of a chemical process, although generally employed simultaneously, are topological and parametric. The topological approach is concerned with the physical layout of the plant. Parametric optimization involves manipulating process variables, such as the temperatures and pressures of certain unit operations. The goals of each approach are the same: maximize the profitability of a process within the given constraints. All process optimization problems start from a base case. The base case can be a simple flow-sheet, a detailed design, or most commonly, a process that is already in operation and needs improvement. The information presented in this work is not intended for the professional in the field, but rather, for a general audience seeking to organize their thoughts regarding chemical process optimization and to provide a basis from which to confront process optimization problems.

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Section 1: Introduction and Purpose

In general, optimization is the improving of any existing situation, including a chemical process.¹ Achieving the optimum operation of a chemical process is an endless task, and the sole purpose of the chemical process engineer. The goal of optimization is to maximize the economic potential of a process, thus all decisions made are based on economics, within certain safety, ethical, and environmental boundaries. Just as the design of a new process is open-ended, so is the continuous optimization of an existing process. Optimization is often misunderstood as a complex, esoteric, manipulation of mathematical equations. In reality, optimization of any process is an open-ended, creative exercise involving brainstorming, exploring alternatives, and continuously asking “what if?”¹ Presented here are a number of approaches that should be considered when confronted with an optimization problem, as well as a sampling of the terms necessary to speak the language of chemical process optimization.

Section 2: Background and Terms

Section 2.1: Objective Functions

The objective function of any optimization is a mathematical function that reaches an extreme value, either maximum or minimum, for the best values of the decision variables, to be covered next. There can be multiple objective functions for a given optimization problem, including profit or cost.¹ Only after an objective function has been chosen can one quantify the optimization process. Since the purpose of optimization is to increase the economic potential of a process, most objective functions have units of dollars. Recurring costs are often discounted to obtain a net present value (NPV). Another option is to annualize capital costs to obtain an equivalent annual operating cost (EAOC).¹ The objective function should be chosen such that an extreme maximum or minimum is the ideal case. For example, minimizing the EAOC and maximizing the NPV are common objectives.

The selection of objective functions is also dependent upon the scope of the optimization. For example, if only one aspect of a process is being optimized that may not have a significant effect on the capital and recurring costs of the rest of the plant. Thus, raw material, capital, and utility costs for the entire plant should not be included here. If they are, then the variation in the EAOC or NPV due only to the variation in the objective function might be dwarfed in comparison to the overall objective function. While the optimization of a single area of a process may not have a great effect on the

overall EAOC or NPV, the downstream effects on the process may. Focusing on individual areas of cost or savings rather than the total cost or savings is termed incremental analysis. Modification to the process continues as long as the return on incremental investments is greater than the MARR.¹

Not all objective functions are directly based on economics, however, the objective function should be quantitative.¹ For example, the objective may be to maximize the production of a chemical or to minimize the concentration of a contaminant in order to comply with environmental regulations. There should always be some rational basis upon which the objective function is chosen. If maximizing profit, not revenues, is the goal, then maximizing production may not be desirable. Likewise, if causing the least amount of harm to the environment is the goal, then minimizing the concentration of contaminant, rather than the total flowrate, may not be the best approach.¹

Section 2.2 Decision Variables

Decision variables, also called design variables, are the independent variable over which the engineer has some control. Decision variables include continuous variables such as temperature and pressure and discrete variables such as the number of trays in a distillation column.¹ Since all realistic optimization problems must be done within a reasonable amount of time, it is necessary to prioritize the decision variables. Those which have the greatest effect on the objective function must receive detailed examinations. Also noteworthy is the fact that raw materials usually account for the vast

majority of recurring costs. Thus, high overall conversion of raw materials and recovery of unreacted raw materials is an essential goal in optimization. Since there are an infinite number of decision variable combinations within a process, knowing the sensitivity of the objective function to changes in the decision variables provides useful insight in to where one's efforts should be focused. For example, if the goal is to increase single-pass conversion through a reactor for which the temperature, pressure, and volume are decision variables, then elaborate mathematical models can be built to estimate the sensitivity of the objective function to each variable. The most efficient technique, however, is to evaluate the objective function at the limits of each variable. If there is little effect on the objective function over the range of possible pressures, then another variable, such as temperature, should be chosen. Many process simulation software tools can evaluate an objective function or dependent decision variable, such as single-pass conversion, over a range of pressures, temperatures, and reactor volumes. Graphs can be generated which show clear trends, or no trend at all if the dependent variable is not very sensitive to changes in the independent variable. More will be said about this later.

Section 2.3 Constraints and the Process Optimum

There are a number of process, ethical, and environmental constraints that may place limitations on the values of decision variables. These constraints may take the form of an equality constraint such as a specific concentration of products leaving a reactor. Mass and energy balances are also equality constraints; the mass entering a system must equal the mass exiting. A constraint may also be an inequality constraint such as a

catalyst that can only operate effectively below 400°C, or below 20 MPa. In general, an equality constraint reduces the number of truly independent decision variables, while an inequality constraint bounds the range over which a decision variable can be evaluated.¹ Constrains may be set by environmental regulations, industry standards, or consumer preferences. Often times, constraints simplify the optimization process by limiting the possibilities that should be evaluated.

Generally, the goal of an optimization problem is to find the extreme value of the objective function for a process. As mentioned above, minimizing the EAOE and maximizing the NPV are common pursuits. A situation when the objective function has been minimized or maximized, whichever is desirable, is termed the *local optimum*. In other words, no small, allowable change in decision variables in any direction will improve the objective function once the local optimum has been reached.¹ It is worth mentioning that nearly all optimization problems of any complexity have local optima at the extreme of at least one constraint. The global optimum, on the other hand, is a situation in which the best objective function exists for all allowable values of the decision variables.¹ A true global optimum will almost certainly defy process constraints. For example, the profit of a plant may be maximized, but if it is producing a hundred tons per day of toxic waste, then this is not an acceptable solution. The global optimum is not a feasible goal, however there are a number of approaches to optimization which will guide the chemical process engineer in that direction.

Section 3: Approaches to Optimization

There are virtually endless possibilities, combinations, and methods when optimizing a chemical process. Presented here are a few approaches which serve as guidelines to organize the chemical engineer's thought process when confronting optimization. Because one can get lost in the minute details of a process, it is vitally important to keep the big picture in mind. While changes in the decision variables must be analyzed, many assumptions can be made that will simplify the optimization process. For example, it is generally assumed that all of the mass that enters a system in a process stream also exits the system via a process stream. In actuality, some mass will be lost by evaporation and through leaks in the system. Focusing on the big picture first, then delving into the process details is called *top-down* optimization. The reverse, or a detailed study of incremental changes leading up to the big picture, is called bottom-up.¹ Both approaches are valid and should ultimately lead to very similar solutions.

All optimization problems dealing with existing processes begin from a base case. It may be a very simple conceptual flow-sheet, a detailed design, or most commonly for the chemical process engineer, an actual plant whose operation one wished to improve. Since the goal of optimization is to improve the process, it is necessary to start from a defined process, that is, a base case.¹ Choose the best available base case either from prior experience, after doing some research into what is effectively used in industry, or what is already in place. Once the base case is chosen, some analysis is necessary to

determine where to begin optimization. At a minimum, the objective function must be calculated. If the objective function includes capital and operating costs, the base case analysis must include equipment sizing and pricing calculations, as well as material and energy balances to determine utility costs. The analysis should clearly show the effect of changes in all important decision variables on the objective function.¹ A sensitivity analysis, covered later, is an effective visual aid in determining which decision variables have the greatest effect on the objective function. It should be reemphasized to not lose sight of the big picture. Virtually every change in process conditions has some downstream effect which must be accounted for. As the engineer practices the approaches presented here, he will sharpen his intuition and what once seemed nontrivial will become second nature.

Essentially, there are two types of optimization: topological and parametric. Topological optimization deals with the physical configuration of the process equipment. Parametric optimization involves manipulating operating conditions, i.e. decision variables, and measuring the effect on the objective function.¹ Most often, these two types of optimization are employed simultaneously, thus, knowledge of both types of optimization is essential.

Section 3.1 Topological Optimization

Whether designing an entirely new process unit, or modifying an existing unit, topological optimization should be considered first. There are two primary reasons for this. First, topological changes to a process typically have the greatest effect on the

overall profitability of the plant. Second, parametric optimization is made easier by having a set topology. When considering the topology of a process, a process engineer should evaluate the following four questions, roughly in the order of which they are presented.

1. Can unwanted by-products be eliminated? Since raw materials are typically the largest expense in a chemical process, obtaining 100% conversion of those materials with 100% selectivity of the desired product is an obvious goal. While almost impossible in practice, such conditions can be approached by use of appropriate reaction mechanisms, reactor conditions, and catalyst. In many cases, catalysts can suppress, but not completely eliminate, side reactions producing unwanted by-products. They are termed *unwanted by-products* because they cannot be sold for an overall profit. An example is a fuel stream. While it can be burned in a boiler to produce steam, which serves as a utility credit, there is a valuable loss in the raw material that was used to produce it.

There are several process changes that may help to eliminate side reactions. Reducing the per-pass conversion of limiting reactant through a reactor can suppress side reactions by reducing the concentration of the reactants which produce unwanted by-products. This is accomplished via a recycle loop flowing from the reactor effluent to the reactor inlet. As the recycle flow rate increases, however, this option becomes more costly. Another option may be to increase the ratio of one reactant to another. For example, consider the general set of reactions:



Unwanted Side Reaction: $2B + C \rightarrow D$

If A is fed to the reactor in sufficient excess of B, the concentration of B in the reactor will be decreased such that the molecular collisions producing the second reaction will be minimized. A third option is to obtain a new catalyst for which the desired reaction is favored more so than with the current catalyst.

Another concern with producing unwanted by-products is environmental regulations. Treatment of streams containing hazardous waste can be extremely expensive and have grave consequences for the profitability of a process. "For many companies, the production of hazardous wastes is no longer an acceptable process choice, and alternative reaction routes, which eliminate such waste streams, are aggressively pursued."

2. *Can equipment be eliminated or rearranged?* Significant improvements in process economics can be achieved by both the elimination and rearrangement of equipment.¹ Here it shall be assumed that all process equipment in the base case serves a valid purpose and that no equipment is redundant and can be eliminated immediately. Generally, it is the changes made to operating conditions, perhaps as a result of parametric optimization, which allow for equipment to be eliminated. For example, consider reducing the per pass conversion of limiting reactant through a reactor as mentioned above. This results in suppression of an unwanted side reaction and thus reduced concentrations of the unwanted by-product downstream. If the resulting concentration of unwanted by-product is below the maximum specification, which could be set by the customer or by environmental regulation, then separation of the final product might be made easier, perhaps allowing for the elimination of a second

distillation column. Note, however, that reducing per pass conversion will require an increase in the recycle flow rate around a reactor. It is possible that this will increase utility costs such that the savings from the elimination of the second distillation tower are washed out, making this option economically unjustifiable. A situation in which the elimination of equipment is justified results in a step change in the economic objective function, shown in Figure 1. Notice that the step change may result in a new optimum.

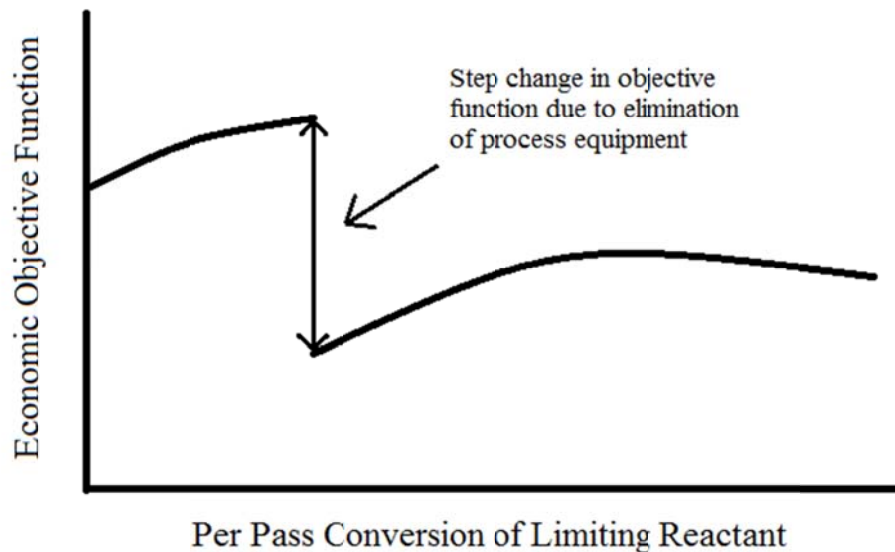


Figure 1: Step change in objective function (NPV) due to elimination of process equipment vs. per pass conversion of limiting reactant.

Rearranging equipment can be equally advantageous to the process economics. Some arrangements are quite trivial, while others may be less obvious. For example, a simple knowledge of thermodynamics suggests that it is easier to pump a liquid than compress a gas. Consequently, it is always better to place a pump before a vaporizer rather than a compressor after it. More subtle are the many possible rearrangements in the separation section of a process. To determine the best separation sequence for a

process, rigorous parametric optimization is typically required, however, there are a few general guidelines which can steer the chemical engineer in that direction. These guidelines¹ should help determine which sequences warrant further investigation:

1. Perform the easiest separation first – that is, the one least demanding of trays and reflux – and leave the most difficult to the last.
2. When neither relative volatility nor feed composition varies widely, remove components one by one as overhead products.
3. When the adjacent ordered components in the feed vary widely in relative volatility, sequence the splits on order of decreasing volatility.
4. When the concentrations in the feed vary widely but the relative volatilities do not, remove the components in order of decreasing concentration.

It is worth noting that these guidelines do not mention exceptions due to a mixture containing water. Because water has a very high latent heat of vaporization compared to organic materials, the distillation of a water containing mixture requires much higher reboiler duties, and therefore is more expensive. Although water may not be the most volatile component in a mixture, separation of water first in a series of distillation columns will decrease the reboiler duties on the successive columns. This may provide an economically justifiable deviation from the guidelines. Special consideration should be given when performing a separation on any mixture of polar or other compounds that may form azeotropes or give rise to more than one liquid phase.¹ The complexity of a separation is greatly increased when the removal of components from a mixture causes the mixture to form two liquid phases. In this case, consideration should be given to the

sequence in which components are removed in order to simplify the separation as much as possible.

3. Can alternative separation methods or reactor configurations be employed?

Employing the most appropriate separation method can drastically improve the economic potential of a process. Since raw materials are typically the largest expense in a chemical process, recovery of unreacted materials is of great concern. There exists a plethora of separation technologies which are available to the chemical process engineer for separation of raw materials and products. Despite this wide range of options, the vast majority of separations in liquid-gas processes are composed of distillation, gas absorption and liquid stripping, and liquid-liquid extraction. Since distillation technology has been effectively used in industry for many years, and because of its relatively inexpensive energy requirements, it is the default option for process separations involving liquids and vapors.¹ Distillation does come with some limitations, however, and the use of alternative separation methods should be considered early on in the design of a process. For example, mixtures containing components with relative volatilities near 1 (less than 1.3 in practice) or if very high pressures or low temperatures are needed to obtain a vapor-liquid mixture. In this case, cryogenic, membrane, or pressure swing adsorption methods may be used. Separation of fuel gases, such as a mixture of methane and hydrogen, require these methods. It should be evaluated whether the increased cost of these methods overshadows the savings. Do remember, though, that raw materials typically make up the greatest cost to a process, and thus are better recycled than used as fuel gas.

Reactor configurations can limit or maximize the conversion of raw materials, and thus have significant effects on economic potential. An in depth approach to reactor configuration is not covered here, but there are four basic effects on reactor performance which the chemical process engineer must consider when designing and optimizing a reaction configuration.

1. *Reaction Kinetics and Thermodynamics:* Extensive variables such as pressure, temperature, and concentration determine the rate of a reaction and its equilibrium. They can also determine the extent of a reaction, or how much reactant can be converted to products, as well as the necessary reactor volume to achieve a given conversion. Catalysts are also used to increase the rate of a reaction, however they do not alter the equilibrium state of a reaction.
2. *Reactor Parameters:* The volume, space time, and reactor configuration affect the extent to which reactants can be converted to products. When designing a reactor, the volume necessary to achieve a certain conversion can be found if the kinetics, thermodynamic, reactor and heat transfer configuration, and space time are given. If a reactor of a given size is available, which is most common in optimizing an existing process, then the temperature, space time, catalyst, and reactor and heat transfer configuration affect the conversion.
3. *Production of Desired Product:* Reactor performance is generally expressed in terms of three parameters: conversion, selectivity, and yield. Single-pass conversion is the ratio of reactant consumed in the reactor to the reactant fed to the reactor. Overall conversion is the ratio of reactant consumed in the

entire process to the reactant fed to the reactor. As previously mentioned, high single-pass reactor conversions are not necessary, and are often times not desirable, for optimum reactor performance. Low single-pass conversions with increased recycle can be utilized to achieve high overall conversions. Selectivity is the ratio of the rate of production of the desired product to the rate of production of undesired by-products. Conversion of the limiting reactant to the desired product is limited by competition from undesired reactions.¹ Yield is the ratio of the moles of reactant reacted to produce the desired product to the moles of limiting reactant reacted. Each of these is a function of reaction kinetics, thus temperature, pressure, reactor and heat transfer configurations, and space time have an effect.

4. *Heat Transfer in Reactor:* In exothermic reactions, heat is generated. The heat must be removed efficiently to prevent hot spots, which can kill the catalyst, and runaway reactions, which occur when the rate at which heat is generated exceeds the rate at which it can be removed. In endothermic reactions, heat is consumed. The heat must be supplied to the reaction efficiently enough so that the reaction may proceed. Otherwise, cold zones may form and the reaction rate will slow. In both cases, the rate of heat transfer is dependent upon the reactor and heat transfer configurations, the properties of the reacting stream and heat transfer medium, and the temperature driving force, which could be affected by temperature gradients.¹

4. *To what extent can heat integration be improved?* Effectively and efficiently designing the heat integration network of reactors and process streams can minimize the

amount of utilities that must be purchased. The basic premise of optimizing process heat integration is to take heat generated in one section of a process, perhaps from an exothermic reaction, and to use it in another section of the process. One method of accomplishing this is to use the heat to produce steam from boiler feed water, which can be used in another part of the process requiring heat, perhaps to vaporize the contents inside the reboiler of a distillation column. In order to minimize the flow rate of the utility stream, a minimum approach temperature should be used, generally around 10°C. This means that the difference in temperature between the inlet of the utility stream and the outlet process stream in a heat exchanger should be at least 10°C. Using a minimum approach temperature ensures the driving force for heat transfer is large enough to be effective without excessive utility stream flow rates. There are methods by which the minimum number of heat exchangers needed in a process can be found, however those methods are outside the scope of this work.

Section 3.2 Parametric Optimization

In order to simplify the optimization of any process, the key decision variables should be identified early in the optimization procedure. Choosing the most appropriate variables for which to spend time drastically increases the efficiency of the optimization process. For most processes, the following list provides a sufficient amount of decision variables to consider.

1. Reactor operating conditions, for example, temperature, pressure, and reactant concentrations. The operational temperature range may be limited by the

catalyst, which could be killed under too much heat, and ineffective with not enough.

2. Single-pass conversion in the reactor. Selectivity of the desired products is a function of the single-pass conversion, which is in turn a function of the parameters mentioned in (1).
3. Recovery of unused reactant.
4. Purge ratios for recycle streams containing inerts.
5. Purity of products, which is often set by market forces such as customer specifications.
6. Reflux ratio and component recovery in columns, as well as the flow rates of mass separating agents in absorbers, strippers, and extraction units.
7. Operating pressures of separation units. Operation below 1 atmosphere is uncommon since this is a partial vacuum compared to the atmosphere, and air is likely to leak into the system.

Virtually any change in process conditions has downstream effects. This applies even to recycle loops, where any change in operating conditions within the loop affects operation of all pieces of equipment in the loop. Process equipment that does not lie in a loop, such as a distillation column which separates a binary mixture of two products, can be considered independently once the upstream process has been optimized. During parametric optimization, it is typical that the topology of the plant remains unchanged, unless the result of optimizing a process condition allows for the elimination of process equipment, as mentioned earlier.

Changes in operating conditions due to parametric optimization often require corresponding changes in utilities.¹ For example, lowering the pressure inside a distillation column to achieve better separation will lower the temperature necessary in the reboiler. This decrease in the required amount of heat may mean a switch to medium pressure steam from high pressure steam, or to low pressure steam from medium pressure steam, is available. Lower pressure steam is less costly and will result in savings and a better economic objective function. A process change which allows for the switch from refrigerated water to cooling water is also desirable. It is worthwhile to remember that utilities account for a large portion of the yearly cost of a plant, thus time is well spent in minimizing their effect on the objective function.

The range over which decision variable should be evaluated is also a valid concern. While the choice of these ranges is somewhat arbitrary, it is good practice to at least evaluate each decision variable at its extreme values. For example, if a catalyst is ineffective below 200°C and begins to sinter above 450°C, then the effects of operating the reactor outside this temperature range should not be considered, but the extreme values should. To minimize the amount of time spent on the process simulation, the number of points evaluated for each variable should be chosen wisely. Simulation software packages, such as Pro II provide sufficient relief from this time concern, if they are available to the engineer. The *case study* function allows an independent variable, such as reactor temperature, to be varied over a given range and the effect on the dependent variable, or objective function, is represented by graphs or tables which may clearly show local maxima or minima. A global optimum is virtually impossible. In this situation, any change in process conditions would lead to inferior process performance.

Another optimization tool that can help direct where the most time should be spent is a sensitivity analysis, which measures the sensitivity of the objective function to changes in decision variables. A sensitivity analysis can be constructed by changing one decision variable while keeping all others constant, and observing the effect on the objective function. This can be a very effective visual tool for conveying which decision variable should receive the most attention. Figure 2 shows an arbitrary sensitivity analysis. Notice that the greatest effect on the estimated NPV occurs when the sales price of the product is varied. This is, however, generally tied to market forces, thus the engineer may have no control over this parameter. Raw materials cost, on the other hand, can be effectively lowered by optimization, either by achieving better conversion and selectivity of the desired product, or by recovering more unreacted raw materials. In most chemical processes, the NPV is most sensitive to the cost of raw materials. For the arbitrary case, utility and equipment costs have little effect on the NPV, primarily because they represent only a small portion of the cost of the process.

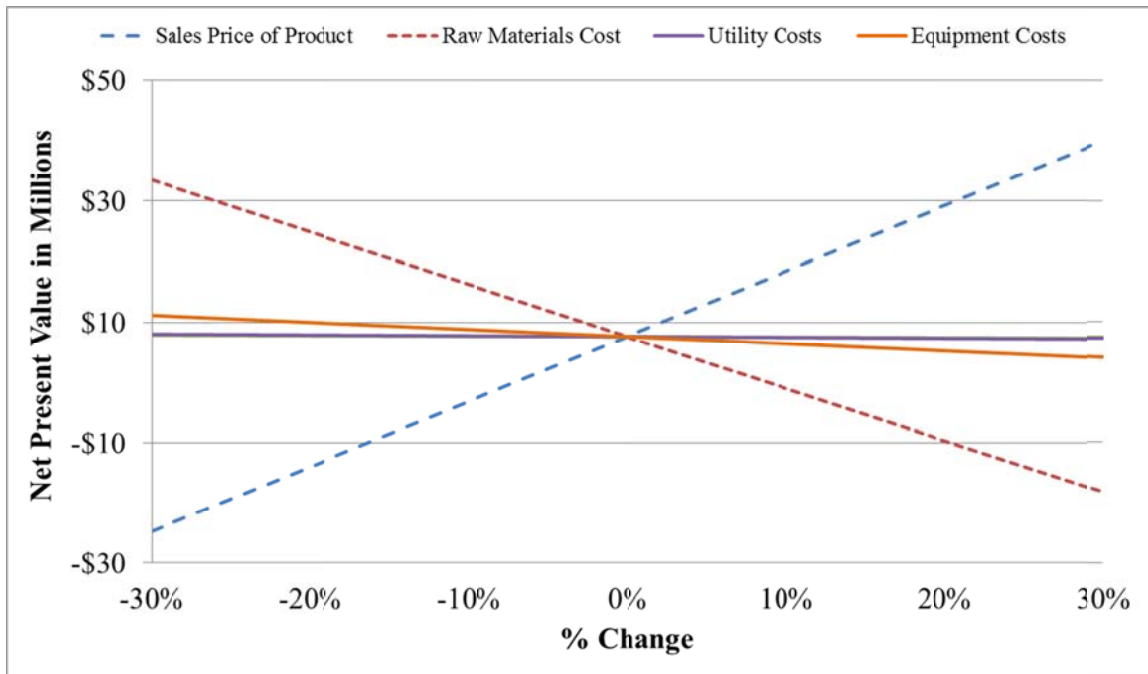


Figure 2: Sensitivity analysis of an arbitrary process. Each line represents a percent change in the respective parameter while holding all other parameters constant. Note: the NPV is most sensitive to the raw materials cost and the sales price of the product.

Section 4: Conclusions

The chemical engineer has a multitude of tools with which he can approach an optimization problem, topological and parametric approaches included. While reaching a global optimum is infeasible, approaching the most economically favorable process is an endless pursuit. While chemical processes are most often presented as steady-state processes, in reality, they are constantly in flux. Process equipment must be able to operate under a range of conditions, such as different feedstocks, varying weather conditions (especially important for cooling utilities), over a range of catalyst activities, and at different production rates, just to name a few.¹ The optimum conditions for the design or base case are most certainly not the optimum for other operating conditions and, in fact, might be extremely inefficient. It is the engineer's job to understand the process with enough depth to effectively make changes to process conditions, troubleshoot, and scale up or down in order to approach an optimum. One must never lose sight of the goal of optimization: to safely, efficiently, and ethically maximize the profit of a business.

Section 5: Example: Utility Optimization

The following example has been adapted from a case study on an ethylbenzene production facility. The premise of this example is heat integration. A process stream containing heat from a highly exothermic reaction enters the heat recover section of a plant before entering the separation section, where the products, by-products, and unreacted raw materials are separated. Typically, the medium with which heat is transferred throughout a plant is steam. When steam must be purchased for use in a chemical process, it is available in three types: high pressure, medium pressure, and low pressure steam (HPS, MPS, and LPS, respectively). The prices, temperatures, and pressures at which steam is available are shown in Table 1. HPS is the most expensive not because it contains the most energy, but because of how it is generated onsite. In fact, LPS contains the most energy on a per mass basis due to its higher enthalpy of vaporization. When steam can be produced using heat from elsewhere within a process, less steam must be purchased, thus, the steam produced can be viewed as a utility credit. It has been assumed in this example that all steam produced may serve a valid purpose, which is not always the case in reality. If there is no use for HPS within a process, then it is not economically justifiable to put forth the capital cost to purchase a HPS producing heat exchanger.

Table 1: Types of steam utility available for purchase and the prices, temperatures, and pressures at which they are available.

	Price (\$/GJ)	Temperature (°C)	Pressure (barg)
HPS	17.70	254	41
MPS	14.83	184	10
LPS	14.05	160	5

For the sake of simplicity, we shall assume that the stream entering the heat recovery section of the plant is approximately 90% ethylbenzene, and 10% unreacted benzene. The base case PFD is shown in Figure 3. The process stream enters the heat recovery section at 458°C. Some heat from that stream is used to vaporize boiler feed water (bfw) into HPS in E-303. The HPS is to be used elsewhere in the process. The process stream, now at 280°C, is then used to produce LPS from bfw in E-304. The process stream, exiting E-304 at 170°C, is then cooled, using cooling water, to 83°C, the temperature of the separation section of the plant.

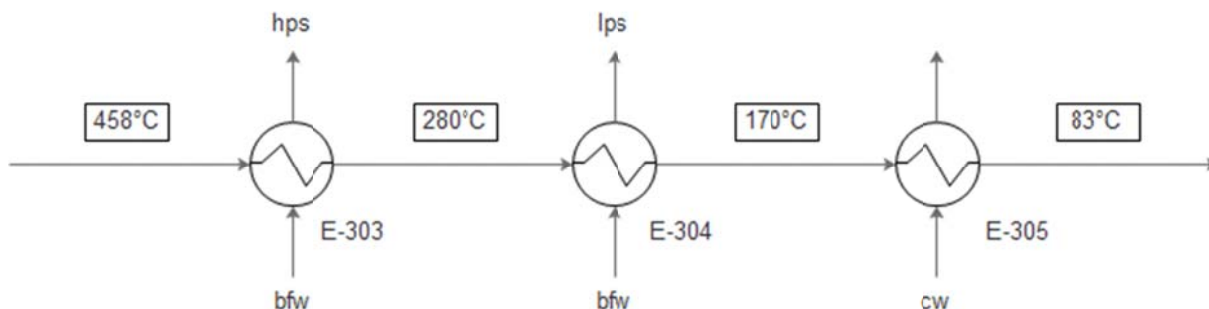


Figure 3: Base case heat recovery section which recovers heat from the highly exothermic reaction and prepares process stream for the separation section. The heat is used to vaporize bfw and the steam is sent to other areas of the process, where it releases the heat, condenses, and is recycled as bfw.

Attention should again be called to Table 1. The higher pressure, higher temperature steam has more value. Therefore, it is only trivial to assume that as much HPS as possible should be produced, then as much MPS, and LPS, in that order. At this point, the chemical process engineer should notice that there is enough heat in the stream leaving E-303 to produce MPS. While this does require expending the capital cost of a new heat exchanger to produce MPS, the increased steam credit, due to the 78¢ difference per GJ in producing MPS over LPS, may outweigh the heat exchanger capital cost over the lifetime of the project. Figure 4 shows a proposed heat recovery section, where a MPS producing heat exchanger is included. A 10°C approach temperature has been assumed. Physically, this means that since the HPS exiting E-303 is at 254°C, then the process stream must exit with a temperature of at least 264°C. This ensures that the driving force for heat transfer, which is temperature difference, is great enough to be effective.

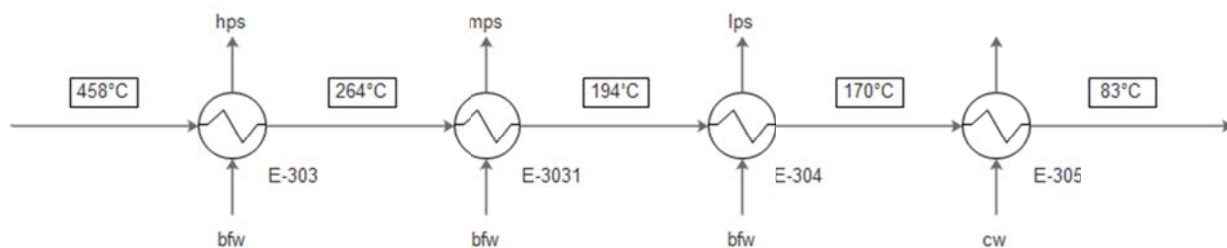


Figure 4: Proposed heat recovery section in which a heat exchanger producing MPS has been added. The inlet and outlet conditions of the process stream through the heat recovery section remain the same.

Since the process stream exiting E-303 is leaving 16°C lower in the proposed case, the area for heat exchange should be larger than in the base case. For the sake of simplicity, we shall assume that E-303 was oversized in the original design to account for a range of operating conditions. Following the same logic, the area of E-304 in the proposed case should be smaller compared to the base case, and the area of E-305 should remain the same. Based on these arguments, we can safely assume no heat exchanger purchases were necessary aside from E-3031, the new MPS producing heat exchanger.

The total module cost (TMC) of E-3031 is approximately \$237k. Here, TMC must be used because the heat exchanger is an addition to an existing plant. Installation fees and special considerations for high pressures and temperatures are accounted for in the TMC. Bare module cost should be used when only the price of a piece of equipment, including any special considerations for high pressures or temperatures, is needed. The additional income earned as a result of producing MPS over LPS accounts to \$25k per year. In order to decide if the \$25k annuity outweighs the \$237k capital expenditure associated with buying a new heat exchanger, these two cash flows must be fairly

compared. Figure 5 shows this comparison. A MARR of 8% has been assumed. The NPV of the annuity is shown as a function of the project lifetime and the NPV of the TMC does not change since that expenditure occurs at the present time. The intersection of these two lines represents the breakeven point, or the time at which the NPV of the annuity equals the TMC of the heat exchanger. Based on this analysis, the purchase of a new MPS producing heat exchanger is economically justified if the lifetime of the project exceeds ~18.5 years. For reference, there are many chemical plants in the United States that are much older than 18.5 years.

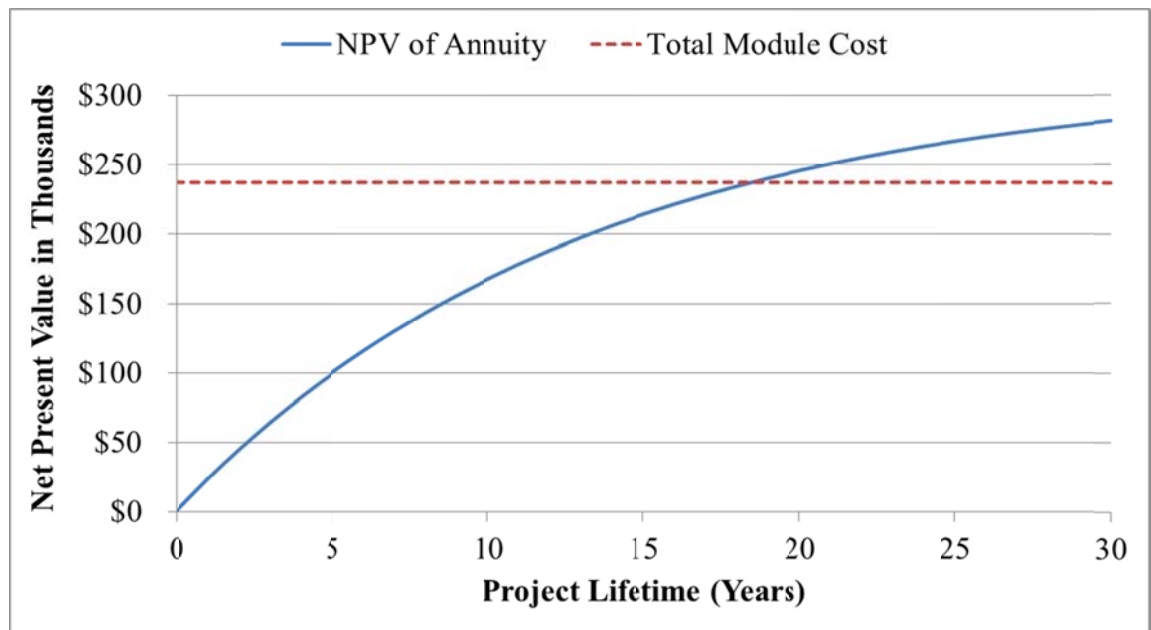


Figure 5: Comparison of the NPV of the annuity and the total module cost of the new MPS heat exchanger vs. the project lifetime.

If the MARR were to increase, the NPV of the annuity would decrease at each instant in time, thus the breakeven point would be pushed further back. This example

illustrates how process design and optimization decisions are made based on economics.

A number of constraints must be met and some assumptions must be made, but ultimately, options can be fairly compared in order to choose whichever provides the greatest increase in the economic potential of a process.

Section 6: References

1. Turton et al. *Analysis, Synthesis, and Design of Chemical Processes*. 3rd Edition.

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